

Coloring random graphs

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(Dated: February 1, 2008)

We study the graph coloring problem over random graphs of finite average connectivity c . Given a number q of available colors, we find that graphs with low connectivity admit almost always a proper coloring whereas graphs with high connectivity are uncolorable. Depending on q , we find the precise value of the critical average connectivity c_q . Moreover, we show that below c_q there exist a clustering phase $c \in [c_d, c_q]$ in which ground states spontaneously divide into an exponential number of clusters and where the proliferation of metastable states is responsible for the onset of complexity in local search algorithms.

PACS numbers: 89.20.Ff, 75.10.Nr, 05.70.Fh, 02.70.-c

The Graph Coloring problem (COL) is a very basic and famous problems in combinatorics [1] and in statistical physics [2]. Given a graph, or a lattice, and given a number q of available colors, the problem consists in finding a coloring of vertices such that no two neighboring vertices have the same color. The minimally needed number of colors is the *chromatic number* of the graph.

For planar graphs there exists a famous theorem [3] showing that four colors are sufficient, and that a coloring can be found by an efficient algorithm. On the contrary, for general graphs the problem is computationally hard to solve: already in 1972 it was shown that Graph Coloring is NP-complete [4] which means, roughly speaking, that the time required for determining the existence of a proper coloring grows exponentially with the graph size.

In modern computer science, graph coloring is taken as one of the most widely used benchmarks for the evaluation of algorithm performance [5]. The interest in coloring stems from the fact that many real-world combinatorial optimization problems have component sub-problems which can be easily represented as coloring problems. For instance, a classical application is the scheduling of registers in the central processing unit of computers. All variables manipulated by the program are characterized by ranges of times during which their values are left unchanged. Any two variables that change during the same time interval cannot be stored in the same register. One may represent the overall computation by constructing a graph where each variable is associated with a vertex and edges are placed between any two vertices whose corresponding variables change during the same time interval. A proper coloring with a minimal number of colors of this graph provides an optimal scheduling for registers: two variables with the same color will not be connected by an edge and so can be assigned to the same register (since they change in different time intervals).

The q -coloring problem of random graphs represents

a very active field of research in discrete mathematics which constitutes the natural evolution of the percolation theory initiated by Erdős and Rényi in the 50's [6]. One point of contact between computer science and random graph theory arises from the observation that, for large random graphs, there exists a critical average connectivity beyond which the graphs become uncolorable with probability tending to one as the graph size goes to infinity. This transition will be called the q -COL/UNCOL transition throughout this paper. The precise value of the critical connectivity depends of course on the number q of allowed colors and on the ensemble of random graphs under consideration. Graphs generated close to their critical connectivity are extraordinarily hard to color and therefore the study of critical instances is at the same time a well posed mathematical question as well as an algorithmic challenge for the understanding of the onset of computational complexity [7, 8]. The notion of computational complexity refers to worst-case instances and therefore results for a given ensemble of problems might not be of direct relevance. However, on the more practical side, algorithms which are used to solve real-world problems display a huge variability of running times and a theory for their typical-case behavior, on classes of non-trivial random instances, constitutes the natural complement to the worst-case analysis. Similarly to what happens for other famous combinatorial problem, e.g. the satisfiability problem of Boolean formulae, critical random instances of q -coloring (or polynomial mappings to other NP-complete problems) are a popular test-bed for the performance of search algorithms [5].

In physics q -coloring has a direct interpretation as a spin-glass model. A proper coloring of a graph is a zero-energy ground state configuration of a Potts anti-ferromagnet with q -state variables. For most lattices this system is frustrated and displays many equilibrium and out-of-equilibrium features of glasses ('Potts glass').

Here we focus on the q -coloring problem (or Potts anti-ferromagnet) over random graphs of finite average connectivity, given by the $\mathcal{G}_{N,p}$ ensemble (graphs composed of N vertices with edge probability p for every pair of vertices). In the relevant limit of finite connectivity we have to take $p = c/N$ which leads to random graphs with a Poissonian connectivity distribution of mean c .

Two types of questions can be asked. One type is algorithmic, i.e. finding an algorithm that decides whether a given graph is colorable. The other type is more theoretical and amounts to asking whether a typical problem instance is colorable or not and what is the typical structure of the solution space. Here we address the latter question using the so called cavity method [9].

Let us start with reviewing some known results on the q -COL/UNCOL transition on random graphs. One of the first important finite-connectivity results was obtained by Luczak about one decade ago [10]. He proved that the threshold asymptotically grows like $c_q \sim 2q \ln q$ for large numbers of colors, a result, which up to a pre-factor coincides with the outcome of a replica calculation on highly connected graphs [11] ($p = \mathcal{O}(1)$ for large N). For fixed number q of colors, all vertices with less than q neighbors, i.e. of *degree* smaller q , can be colored for sure. The hardest to color structure is thus given by the maximal subgraph having minimal degree at least q , the so-called q -core. Pittel, Spencer and Wormald [12] showed that the emergence of a 2-core coincides with random graph percolation at $c = 1$ [6], and is continuous. For $q \geq 3$, however, the q -core arises discontinuously: For $q = 3$ they found, e.g., that the core emerges at $c \simeq 3.35$ and immediately contains about 27% of all vertices. The existence of this core is, however, not sufficient for uncolorability: The best lower bound for the 3-COL/UNCOL transition is 4.03 [13], numerical results predict a threshold of about 4.7 [14]. The currently best rigorous upper bound is 4.99 [15]. Most recently, a replica symmetric analysis of the problem has been performed [16]. The resulting threshold 5.1 exceeds, however, the rigorous bound, and one has to go beyond replica symmetry. At the level of one-step replica-symmetry breaking (1RSB) we are able to calculate a threshold value $c_3 \simeq 4.69$ which we believe to be exact [17]. We also describe the solution space structure which undergoes a clustering transition at $c_d \simeq 4.42$.

As stated above, the question if a given graph is q -colorable is equivalent to the question if there are zero-energy ground states of the anti-ferromagnetic q -state Potts model defined on the same graph. Denoting the set of all edges by E , the problem can thus be described by the Hamiltonian

$$H = \sum_{(i,j) \in E} \delta(\sigma_i, \sigma_j) \quad (1)$$

with $\delta(\cdot, \cdot)$ denoting the Kronecker symbol. The spins σ_i , $i = 1, \dots, N$, are allowed to take the q values $\{1, \dots, q\}$.

This Hamiltonian counts the number of edges being colored equally on both extremities, a proper coloring of the graph thus has energy zero. In this letter we apply the cavity method in a variant recently developed for finite-connectivity graphs directly at zero temperature [18, 19, 20]. This approach consists of a self-consistent iterative scheme which is believed to be exact over locally tree-like graphs, like the ones we consider here. It includes the possibility of dealing with the existence of many pure states. One has to first evaluate the energy shift of the system due to the addition of a new spin σ_0 . Let us assume for a moment that the new spin is only connected to a single spin, say σ_1 , in the pre-existing graph. Before adding the new site 0, the ground-state energy of the system with fixed σ_1 can be expressed as

$$E_0(\sigma_1) = A - \sum_{\tau=1}^q h_\tau^1 \delta(\tau, \sigma_1) \quad (2)$$

where we have introduced the effective field $\vec{h}^1 = (h_1^1, \dots, h_q^1)$. Note that a $(q-1)$ -dimensional field would be sufficient since one of the q fields above can be absorbed in A . We, however, prefer to work with q field components in order to keep evident the global color symmetry. Connecting σ_0 to σ_1 , and calculating the minimal energy of the enlarged graph with fixed σ_0 , this reads

$$\begin{aligned} E(\sigma_0) &= \min_{\sigma_1} \left(A - \sum_{\tau=1}^q h_\tau^1 \delta(\tau, \sigma_1) + \delta(\sigma_0, \sigma_1) \right) \\ &= A - \omega(\vec{h}^1) - \sum_{\tau=1}^q u_\tau(\vec{h}^1) \delta(\tau, \sigma_0) \end{aligned} \quad (3)$$

with

$$\begin{aligned} \omega(\vec{h}) &= -\min(-h_1, \dots, -h_q) \\ u_\tau(\vec{h}) &= \begin{cases} -1 & \text{if } -h_\tau < -h_1, \dots, -h_{\tau-1}, -h_{\tau+1}, \dots, -h_q \\ 0 & \text{else} \end{cases} \end{aligned} \quad (4)$$

The field $\vec{u}(\vec{h}^1)$ has at most one non-zero component, which takes the value -1 , i.e. $\vec{u}(\vec{h}^1) \in \{\vec{0}, -\vec{e}_1, \dots, -\vec{e}_q\}$ with \vec{e}_τ denoting a unit vector in direction τ .

If the new spin σ_0 is connected to d sites with fields $\vec{h}^1, \dots, \vec{h}^d$, and if these spins were previously uncorrelated (which is the case inside one pure state, cf. the discussion in [9]), the propagated fields can be linearly superposed, $\vec{h}^0 = \sum_{i=1}^d \vec{u}(\vec{h}^i)$. Note that the fields never become positive, which reflects the anti-ferromagnetic character of the model. Colors are suppressed by neighbors carrying this color, they can be favored only by suppressing all other colors. If there would be a single state (replica symmetry), every link (i, j) would carry two propagated fields $\vec{u}_{i \rightarrow j}$ and $\vec{u}_{j \rightarrow i}$ which are determined self-consistently. In case of multiple states, these fields fluctuate from state to state and have to be characterized by a full distribution

$Q_{i \rightarrow j}(\vec{u})$, cf. [9, 20]. Due to the global color symmetry, each of these takes the form

$$Q_{i \rightarrow j}(\vec{u}) = (1 - q\eta_{i \rightarrow j})\delta(\vec{u}) + \eta_{i \rightarrow j} \sum_{\tau=1}^q \delta(\vec{u} + \vec{e}_\tau) \quad (5)$$

and can thus be fully described by the probability $\eta_{i \rightarrow j}$ that any of the colors of vertex j is forbidden by edge (i, j) . Denoting the histogram of all $\eta_{i \rightarrow j}$ by $\rho(\eta)$, the self-consistency equation for the distribution of the $Q_{i \rightarrow j}(\vec{u})$ can be reduced to a simple equation for $\rho(\eta)$ [21],

$$\begin{aligned} \rho(\eta) = & e^{-c} \sum_{d=0}^{\infty} \frac{c^d}{d!} \int_0^{1/q} d\eta_1 \cdots d\eta_d \rho(\eta_1) \cdots \rho(\eta_d) \\ & \times \delta(\eta - f_d(\eta_1, \dots, \eta_d)) \end{aligned} \quad (6)$$

where f_d is simply given by

$$f_d(\eta_1, \dots, \eta_d) = \frac{\sum_{l=0}^{q-1} (-1)^l \binom{q-1}{l} \prod_{i=1}^d [1 - (l+1)\eta_i]}{\sum_{l=0}^{q-1} (-1)^l \binom{q}{l+1} \prod_{i=1}^d [1 - (l+1)\eta_i]} \quad (7)$$

This equation resembles a replica-symmetric self-consistent equation and can be solved numerically using a population dynamical algorithm: We start with an initial population η_1, \dots, η_N of size N which can be easily chosen to be as large as 10^6 to generate high-precision data. This population is updated by iterating the following steps until convergence: (I) Randomly draw a number d from the Poisson distribution $e^{-c}c^d/d!$; (II) Randomly select $d+1$ indices i_0, i_1, \dots, i_d from $\{1, \dots, N\}$; (III) Update the population by replacing η_{i_0} by $f_d(\eta_{i_1}, \dots, \eta_{i_d})$.

One obvious solution of Eq. (7) is the paramagnetic solution $\delta(\eta)$. For small average connectivities c it is even the only one. The appearance of a non-trivial solution coincides with a clustering transition of ground states into an exponentially large number of extensively separated clusters. In spin-glass theory, this transition is called dynamical. Still, $\rho(\eta)$ will contain a non-trivial peak in $\eta = 0$ due to small disconnected subgraphs, dangling ends etc. The weight t of this peak can be computed self-consistently from

$$t = e^{-(1-t)c} \sum_{l=0}^{q-2} \frac{(1-t)^l c^l}{l!}. \quad (8)$$

This equation is quite interesting, since a non-trivial solution forms a necessary condition for Eq. (6) to have a non-trivial solution. In fact [12], the fraction of edges in the q -core is given by $(1 - t_{\min})$ with t_{\min} being the smallest positive solution of Eq. (8). Thus, we also find that the existence of an extensive q -core is necessary for a non-trivial $\rho(\eta)$, and forms a lower bound for the q -COL/UNCOL transition.

Unlike in the case of finite-connectivity p -spin-glasses or, equivalently, random XOR-SAT problems [22, 23, 24],

the existence of a solution $t < 1$ is not sufficient for a non-trivial $\rho(\eta)$ to exist. The latter appears suddenly at the dynamical transition c_d , which can be determined to high precision using the population dynamical algorithm. This solution does not imply uncolorability, but the set of solutions is separated into an exponentially large number of clusters. The logarithm of their number, divided by the graph size N , is called the complexity $\Sigma(c)$ and can be calculated from $\rho(\eta)$, cf. [20]

$$\begin{aligned} \Sigma(c) = & e^{-c} \sum_{d=1}^{\infty} \frac{c^d}{d!} \int d\eta_1 \cdots d\eta_d \rho(\eta_1) \cdots \rho(\eta_d) \\ & \times \ln \left(\sum_{l=0}^{q-1} (-1)^l \binom{q}{l+1} \prod_{i=1}^d [1 - (l+1)\eta_i] \right) \\ & - \frac{c}{2} \int d\eta_1 d\eta_2 \rho(\eta_1) \rho(\eta_2) \ln(1 - q\eta_1\eta_2). \end{aligned} \quad (9)$$

The full derivation will be given in [25]. At the dynamical threshold, this complexity starts discontinuously with a positive value, see Fig. 1, and decreases when c is increased. The static RSB transition, and thus the q -COL/UNCOL threshold c_q , are given by the point of vanishing complexity. At this point the number of clusters becomes sub-exponential, and disappears beyond c_q .

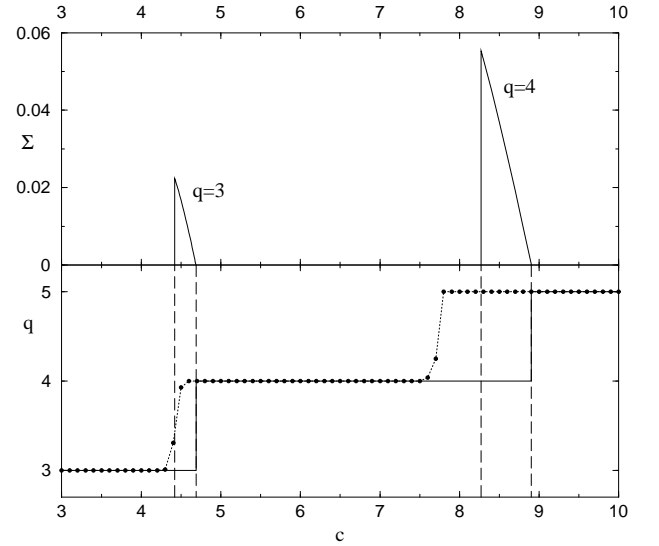


FIG. 1: Top: Complexity $\Sigma(c)$ vs. average connectivity for $q = 3$ and $q = 4$. Non-zero complexity appears discontinuously at the dynamical threshold c_d , and goes down continuously to zero at the q -COL/UNCOL transition. The curves are calculated using the population-dynamical solution for $\rho(\eta)$ with population size $N = 10^6$.

Bottom: The full line shows the chromatic number of large random graphs vs. their connectivity c . The symbols give results of *smallk* for $N = 10^3$, each averaged over 100 samples.

In the following table, we present the results for $q = 3, 4$, and 5. For the dynamical transition we

show the corresponding values of c_d , of the entropy $s(c_d) = \ln q + \frac{\varepsilon}{2} \ln \frac{q-1}{q}$ and the complexity $\Sigma(c_d)$. For the q -COL/UNCOL transition, the critical connectivity c_q and the solution entropy are given. Like in random 3-satisfiability [26] and vertex covering [27], this entropy is found to be finite at the transition point.

q	c_d	$s(c_d)$	$\Sigma(c_d)$	c_q	$s(c_q)$
3	4.42	0.203	0.0223	4.69	0.148
4	8.27	0.197	0.0553	8.90	0.106
5	12.67	0.196	0.0794	13.69	0.082

One can see that the complexity at the dynamical threshold grows strongly with q , whereas the total entropy decreases slowly. This means that the clustering phenomenon becomes more and more pronounced, the number of clusters increases, their internal entropy $s(c) - \Sigma(c)$ becomes smaller. It also becomes more relevant for small systems. At $N = 100$ and the dynamical threshold, we would predict only around 10 clusters for $q = 3$, for $q = 4$ this number would already be close to 250, and grow to about 2800 for 5 colors.

The dynamical transition is not only characterized by a sudden clustering of ground states, at the same point an exponential number of meta-stable states of positive energy appears [20]. Such states are expected to act as traps for local search algorithms causing an exponential slowing down of the search process. Well known examples of search processes that are overwhelmed by the presence of excited states are simulated annealing or greedy algorithms based on local information.

To test this prediction, we have applied several of the best solvers for COL and SAT problems available in the net [5, 28]. The best results could be obtained using the complete *smallk* program [28] which may need exponential time to find a proper minimal coloring. Using a cutoff time (we probed with 10 seconds, 1 minute and 2 minutes without substantial changes for $N = 10^3$), the algorithm can be restricted to sub-exponential times, i.e. only the underlying polynomial-time heuristic is applied. The results in Fig. 1 were obtained in the following way: We first tried to color a random graph ($N = 10^3$) with a small number of colors (here $q = 3$). If, after the cutoff time, *smallk* did not find a coloring, we stopped and retried with larger q . For each connectivity we averaged over 100 samples. As it can be clearly seen, the algorithm fails with q colors slightly below the dynamical transition, confirming our expectations. Only a perfect local heuristic should reach this threshold.

We conclude by noticing that, in similarity to the 3-SAT problem [20], we expect the assumptions underlying the cavity approach to hold for single instances of COL. The equations for the order parameter on single instances provide the full histogram of the N probability distributions of the effective fields, one for each variable, which describe the fluctuations of the polarization of each Potts

variable in the ground states. On the physics side, this information allows to develop a single sample statistical mechanics analysis whereas on the algorithmic side it allows develop new algorithms [25].

We are grateful to A. Braunstein, J. Culberson and F. Ricci-Tersenghi for interesting discussions.

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